

1. A method for use in deriving fixed bond information, comprising: analyzing a delocalized representation of a chemical structure; determining, based on a table of electronic state and valence/distributions,

electronic and bonding characteristics for at least one atom in the chemical structure; and

producing, based the electronic and bonding characteristics, a fixed bond representation of the chemical structure.

2. A system for use in deriving fixed bond information, comprising:

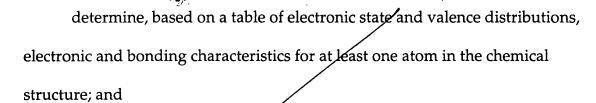
an analyzer analyzing a delocalized representation of a chemical structure;

a determiner determining, based on a table of electronic state and valence
distributions, electronic and bonding characteristics for at least one atom in the
chemical structure; and

a producer producing, based the electronic and bonding characteristics, a fixed bond representation of the chemical structure.

3. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a delocalized representation of a chemical structure;



produce, based the electronic and bonding characteristics, a fixed bond representation of the chemical structure.

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